

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071516\
 Data File : BF089033.D
 Acq On : 15 Jul 2016 23:33
 Operator : UM/SJ
 Sample : H4073-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-01

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.655	5	6	10	rVB	101451	117127	9.04%	0.967%
2	1.770	15	16	24	rVB	825707	1211667	93.55%	10.006%
3	4.821	281	283	287	rBV	57080	78856	6.09%	0.651%
4	5.267	320	322	325	rBV	948408	1138564	87.91%	9.402%
5	6.330	412	415	417	rVB	1232595	1295164	100.00%	10.695%
6	6.444	423	425	427	rBV	1308956	1179494	91.07%	9.740%
7	6.673	443	445	447	rBB	437748	359233	27.74%	2.967%
8	6.833	456	459	461	rBV	1092124	963059	74.36%	7.953%
9	7.245	492	495	497	rBV	824575	822931	63.54%	6.796%
10	7.965	555	558	560	rBV	446860	463949	35.82%	3.831%
11	9.039	649	652	654	rBV	1417357	1176600	90.85%	9.716%
12	9.439	684	687	689	rVB	189878	197013	15.21%	1.627%
13	9.713	708	711	713	rBB	373249	441273	34.07%	3.644%
14	9.805	717	719	721	rBB	26386	18606	1.44%	0.154%
15	10.159	744	750	751	rBB	16950	21342	1.65%	0.176%
16	10.376	766	769	772	rBV2	9342	14243	1.10%	0.118%
17	10.491	777	779	782	rBV	575505	539928	41.69%	4.459%
18	10.628	789	791	796	rBV	29878	37768	2.92%	0.312%
19	11.073	828	830	831	rBV	22174	20572	1.59%	0.170%
20	11.188	837	840	842	rBV	302746	362107	27.96%	2.990%
21	11.428	859	861	865	rVB	21203	27895	2.15%	0.230%
22	12.251	931	933	935	rBV	23556	30820	2.38%	0.255%
23	12.765	975	978	980	rBV	890272	760076	58.69%	6.277%
24	13.679	1056	1058	1062	rBV	50692	65289	5.04%	0.539%
25	13.805	1066	1069	1071	rBV	395201	348290	26.89%	2.876%
26	14.308	1110	1113	1116	rBV	11172	24361	1.88%	0.201%
27	14.525	1129	1132	1134	rBV	11891	15245	1.18%	0.126%
28	14.594	1134	1138	1141	rVV3	5665	19092	1.47%	0.158%
29	14.651	1141	1143	1147	rVB	83764	82525	6.37%	0.681%
30	14.891	1161	1164	1165	rBV	10921	13743	1.06%	0.113%
31	15.165	1185	1188	1191	rBV	216295	233567	18.03%	1.929%
32	15.600	1223	1226	1229	rBV	19313	29042	2.24%	0.240%

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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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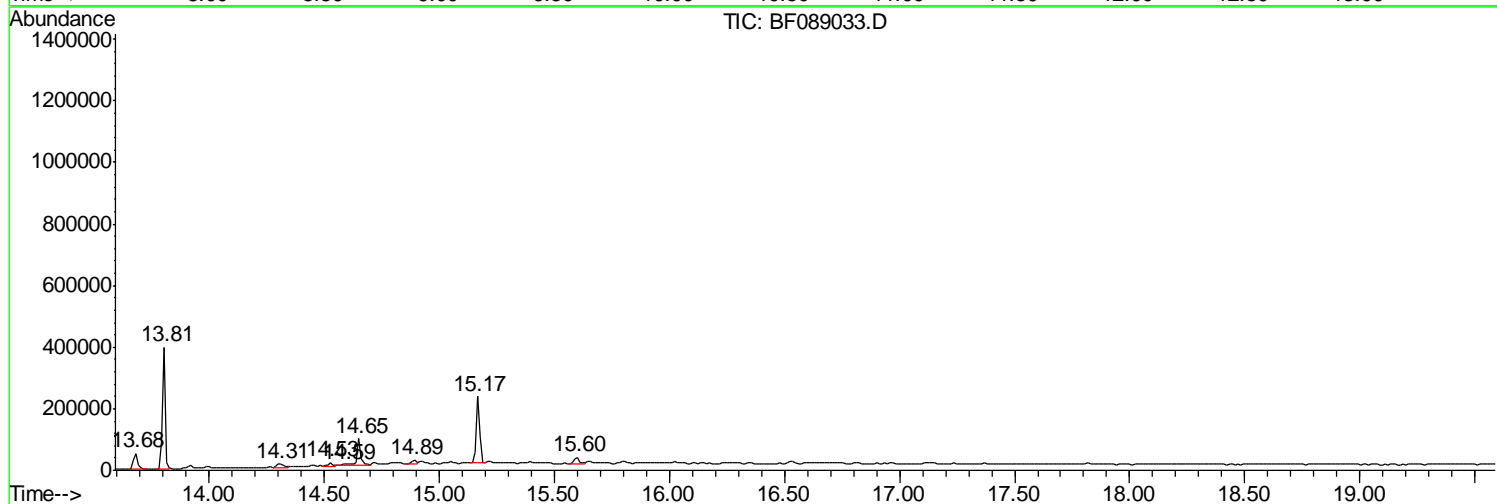
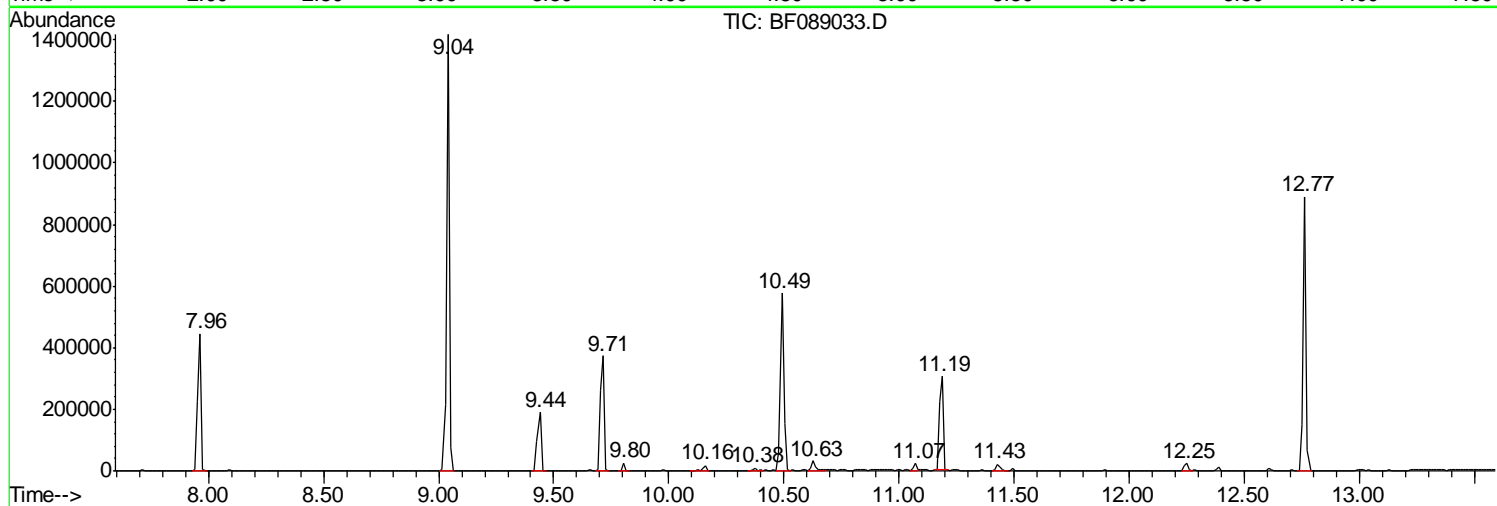
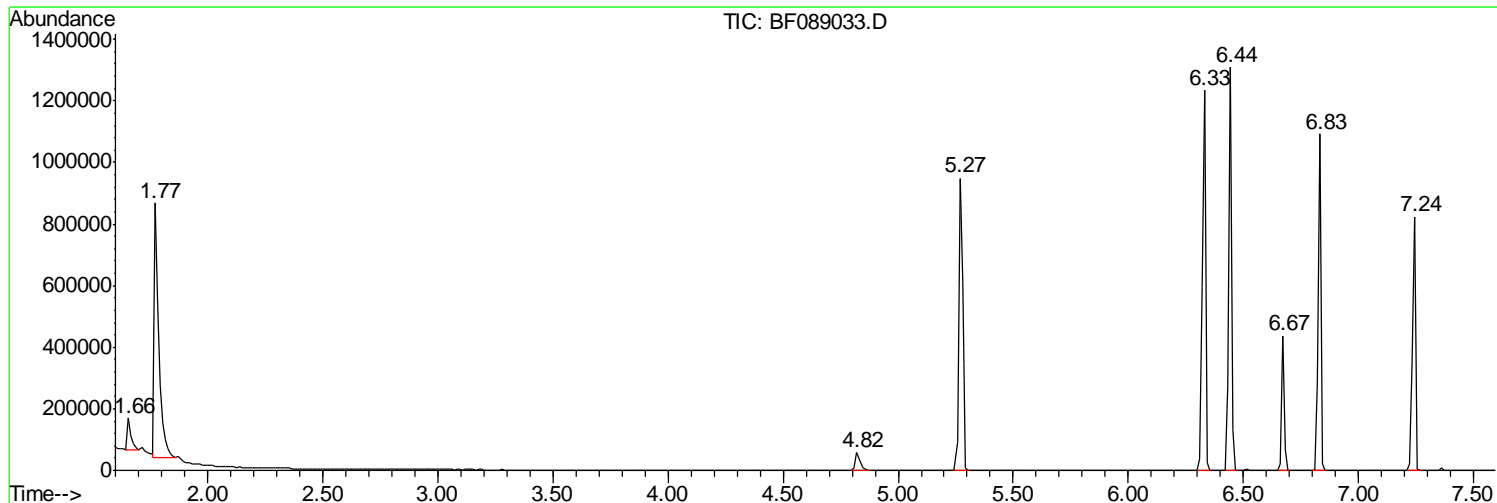
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P



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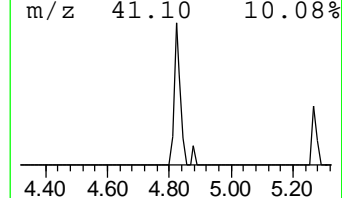
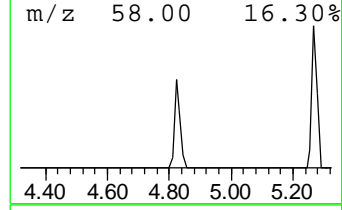
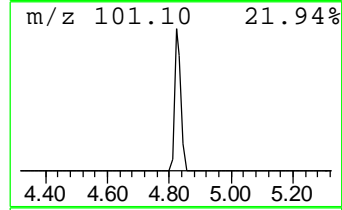
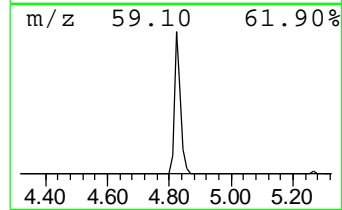
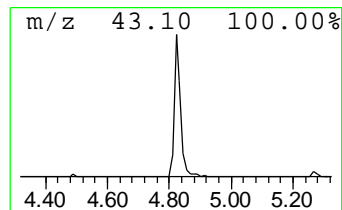
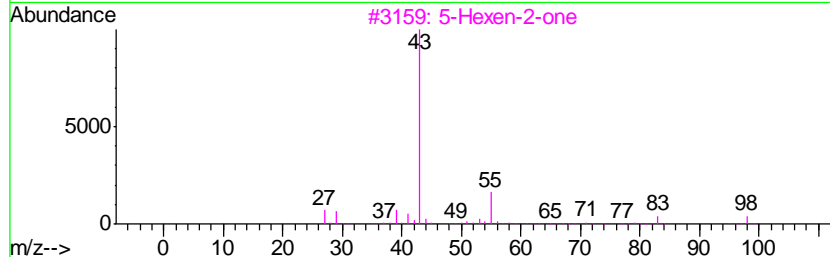
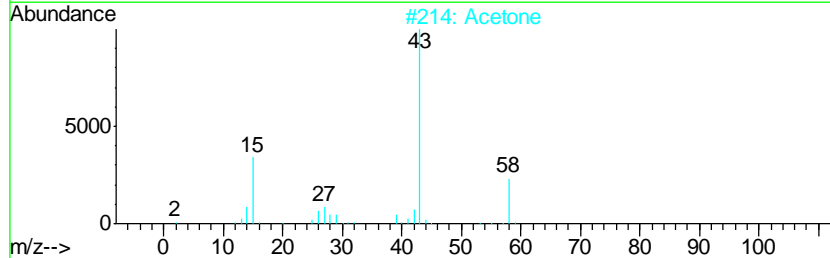
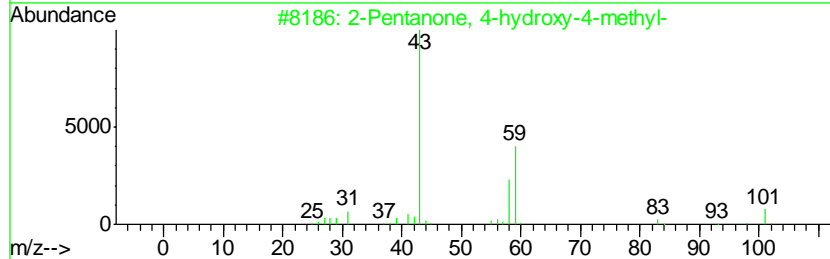
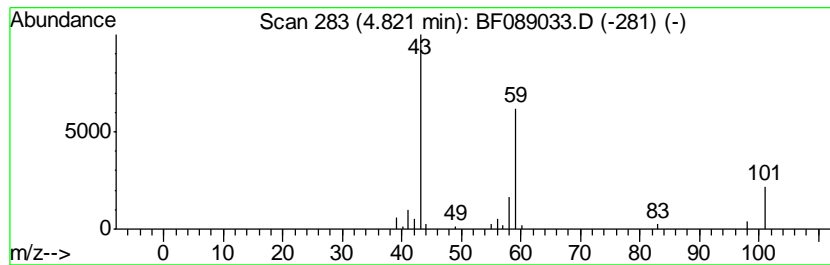
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TIC Library : C:\Database\NIST11.L
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 Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	4.39 ng	78856	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetone	58	C3H6O	000067-64-1	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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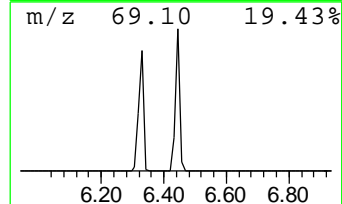
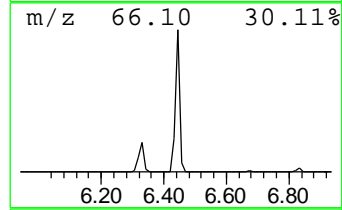
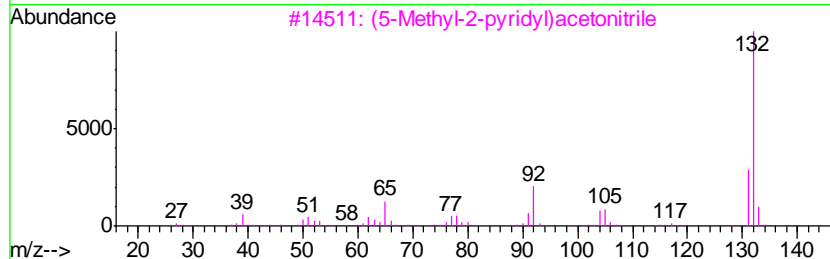
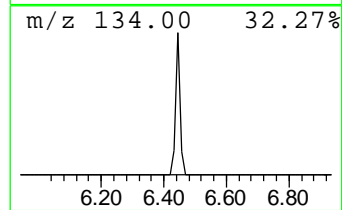
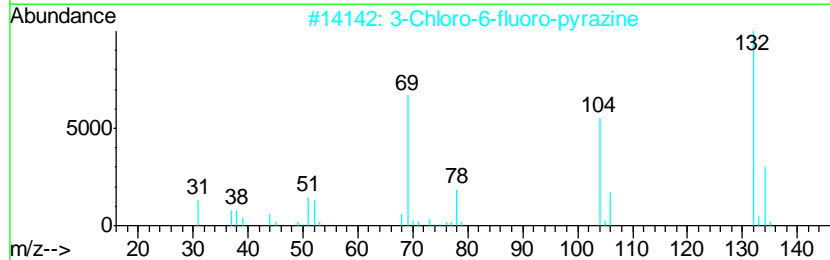
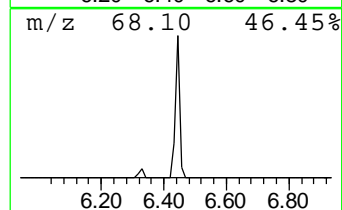
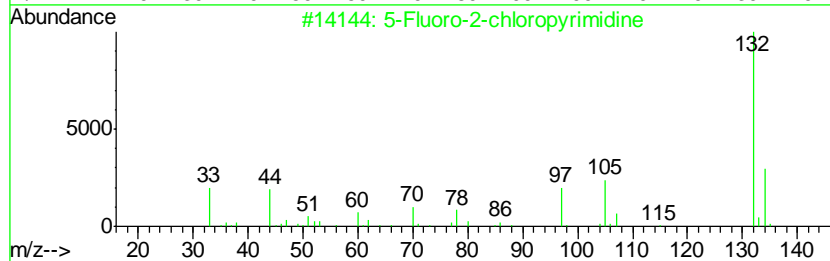
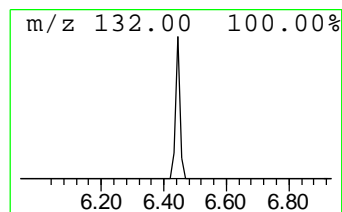
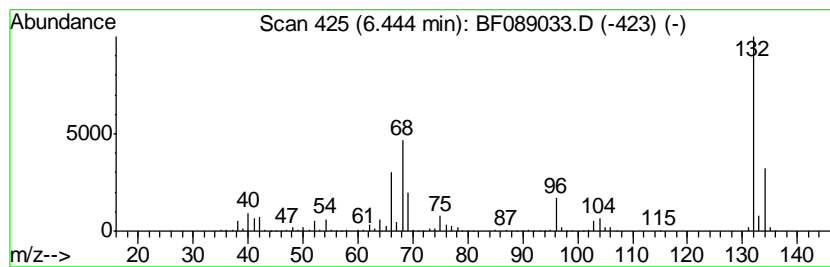
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	65.67 ng	1179490	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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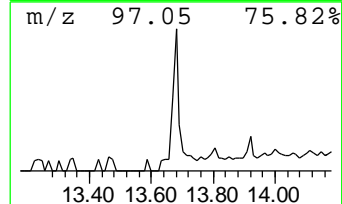
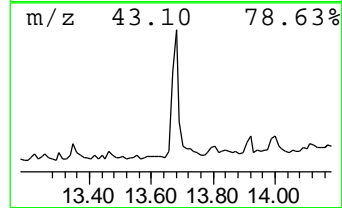
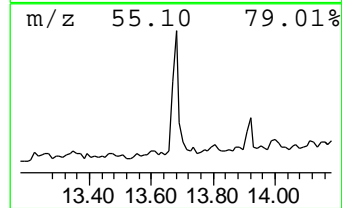
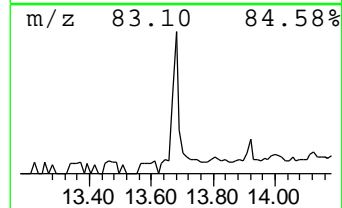
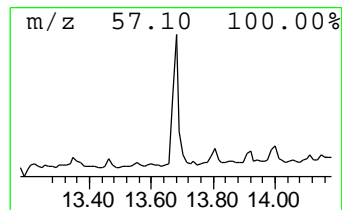
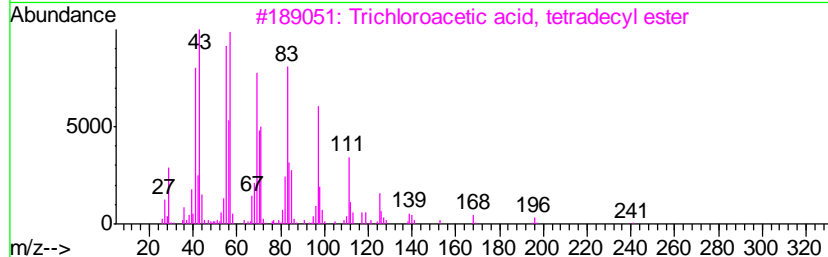
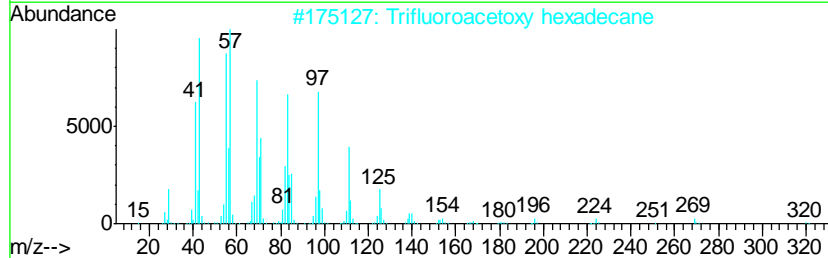
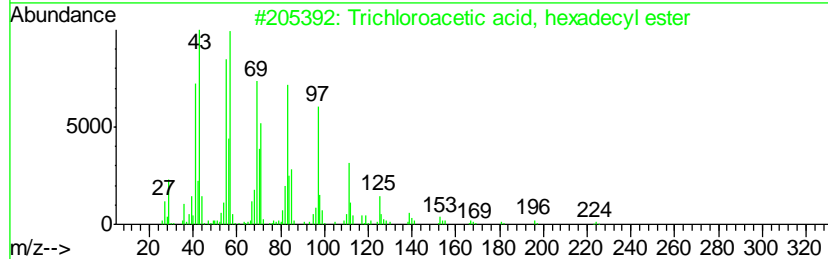
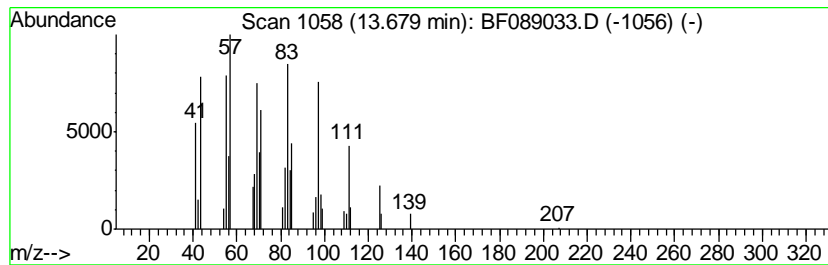
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TIC Library : C:\Database\NIST11.L
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 Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.75 ng	65289	Chrysene-d12	13.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5		1-Heneicosanol	312	C21H44O	015594-90-8	90



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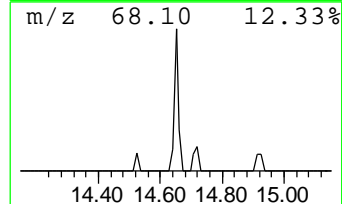
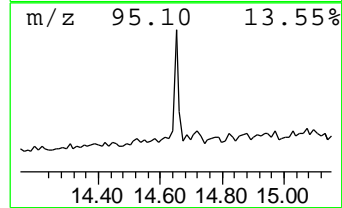
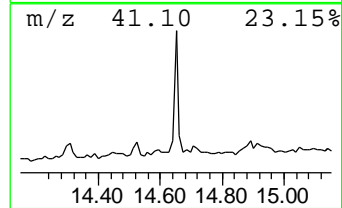
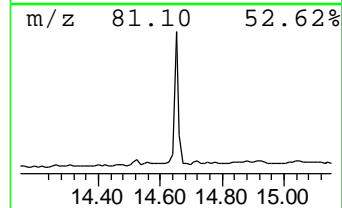
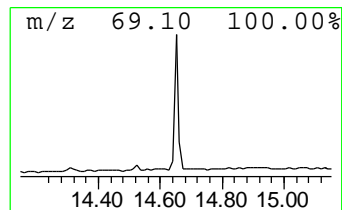
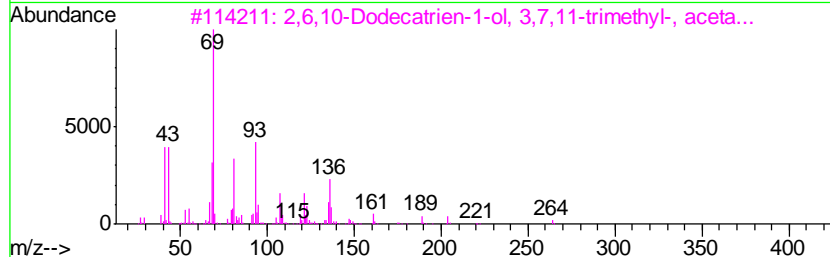
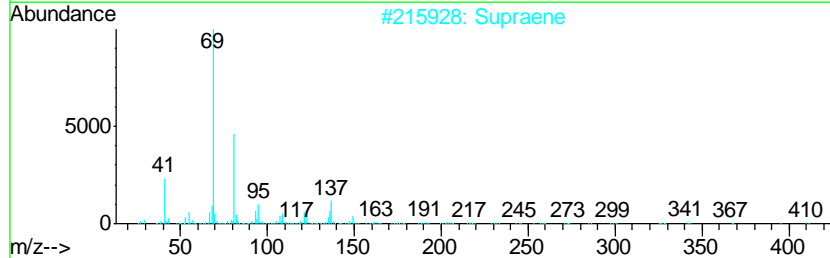
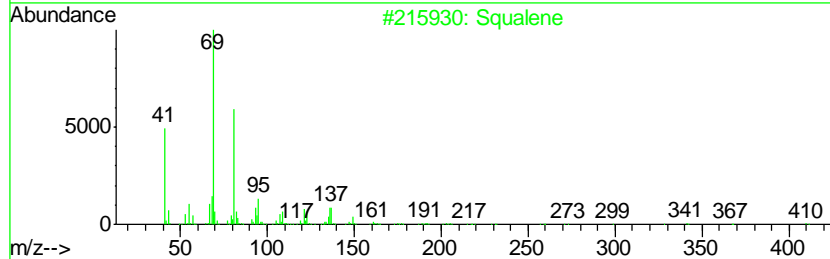
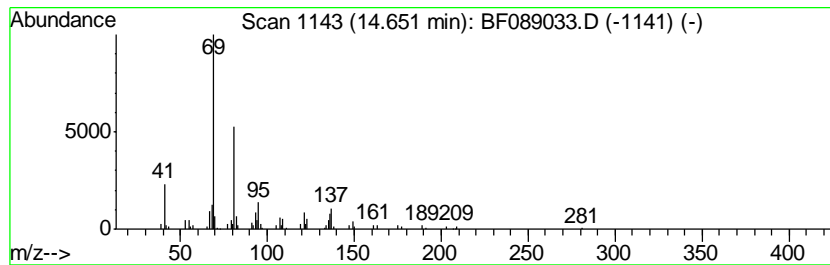
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TIC Library : C:\Database\NIST11.L
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 Peak Number 8 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	7.07 ng	82525	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72
4		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5		Trideca-1,3,7,11-tetraene-1,1-di...	268	C18H24N2	1000159-88-9	59



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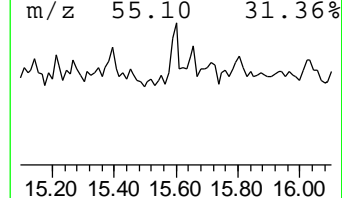
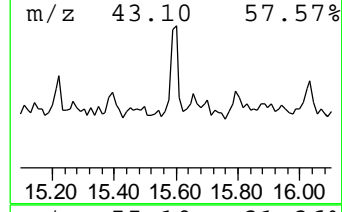
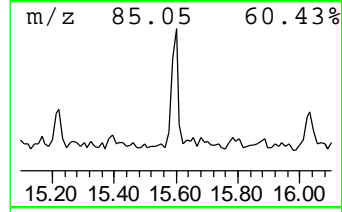
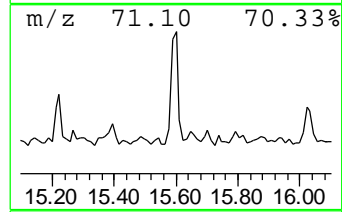
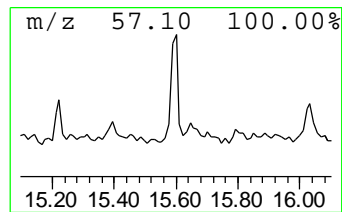
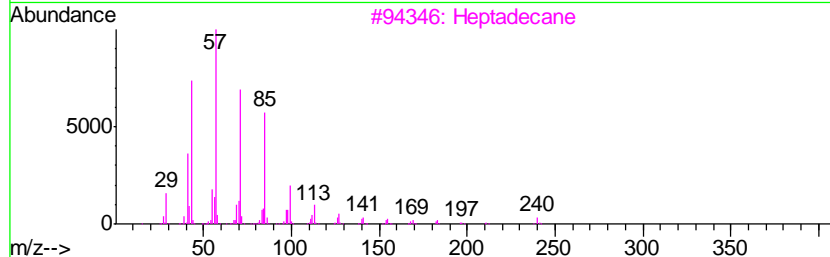
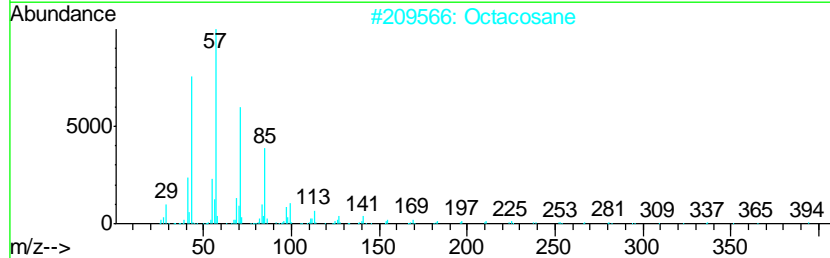
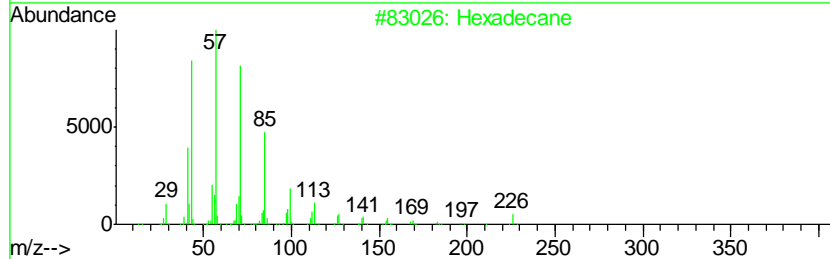
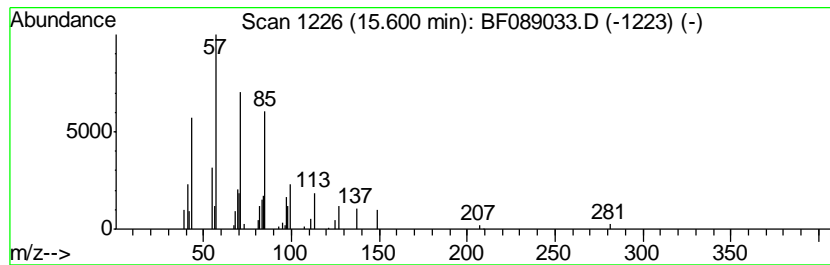
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 Peak Number 9 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.49 ng	29042	Perylene-d12	15.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	64
2		Octacosane	394	C28H58	000630-02-4	64
3		Heptadecane	240	C17H36	000629-78-7	64
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
5		Dodecane	170	C12H26	000112-40-3	59



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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.82	4.4	ng	78856	1	6.67	359233	20.0
unknown6.44	6.44	65.7	ng	1179490	1	6.67	359233	20.0
Trichloroacetic a...	13.68	3.8	ng	65289	5	13.81	348290	20.0
Squalene	14.65	7.1	ng	82525	6	15.17	233567	20.0
Hexadecane	15.60	2.5	ng	29042	6	15.17	233567	20.0